Quantum Interference Effects in Electronic Transport through Nanotube Contacts

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Quantum interference has dramatic effects on electronic transport through nanotube contacts. In optimal configuration the intertube conductance can approach that of a perfect nanotube ($4e^2/h$). The maximum conductance increases rapidly with the contact length up to 10 nm, beyond which it exhibits long wavelength oscillations. This is attributed to the resonant cavity-like interference phenomena in the contact region. For two concentric nanotubes symmetry breaking can reduce the maximum intertube conductance from $4e^2/h$ to $2e^2/h$. The phenomena discussed here can serve as a foundation for building nanotube electronic circuits and high speed nanoscale electromechanical devices.

Carbon nanotubes have electronic and mechanic properties [1] that make them excellent candidates for nanoscale electronic circuits. Simple devices such as diodes [2], single electron transistors [3, 4], field effect transistors [5, 6] and elementary electronic circuits [7] have been built. Understanding the electronic transport through nanotube contacts will be essential for more complex nanotube circuits. Several nanotube/metal contacts [8, 9, 10, 11] and intra-nanotube junctions [12, 13, 14, 15, 16, 17, 18, 19] have been studied theoretically and experimentally. The possibility of using nanotube/nanotube contacts for electronic devices has been suggested [20, 21, 22, 23, 24]. In this paper we examine the electronic transport between two nanotubes, in parallel and in concentric geometries. The variation of conductance with the tube chirality and the contact length is investigated. Characteristic rapid oscillations in conductance, related to the nanotube atomic structure and the Fermi wavelength of the conduction band, are found[21]. In general the inter-tube conductance is small when two tubes have different chirality. However, for *armchair/armchair* or *zigzag/zigzag* the contact conductance is significant and can approach $4e^2/h$ (the conductance of a perfect nanotube) when the contact length is of the order of 10 nm. Further increase in contact length reveals long wavelength oscillations. This is attributed to the quantum interference of the wavefunction in the contact region, which creates resonant cavity-like states. Such oscillations were found in a recent STM experiment [25]. For two concentric nanotubes it is found that the maximum intertube conductance is either $4e^2/h$ or $2e^2/h$ depending on the symmetry of the nanotubes.

The electronic structure of the nanotubes is modeled by a simple π-orbital tight binding hamiltonian[1], taking into account the nanotube curvature. The quantum conductance is calculated using the Landauer-Büttiker formula, with a recursive Green-functions technique [15, 21]. This approach has been shown to provide good agreement with experimentally measured electronic structure and transport properties [15, 21, 25, 26]. Electron-electron interactions play an important role in electronic transport through carbon nanotubes [27], however they have little effect on conductance when the contacts with the leads are highly transparent [28]. In our model the leads are perfect nanotubes to insure good contact with the structure being investigated, therefore electron-electron interactions are not included in the present calculations.

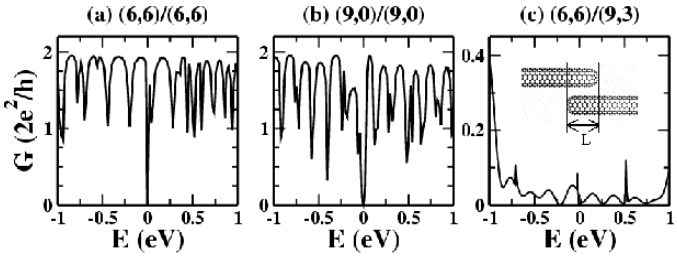

FIG. 1: Intertube conductance for a (a) (6,6)/(6,6) (b) (9,0)/(9,0) (c) (6,6)/(9,3) parallel contact as a function of energy for contact lengths (denoted L on the graph) of order of 10 nm. Notice the presence of a small gap at $E = 0eV$ in (a) and (b) due to interaction between nanotubes. For the same reason the graphs are not symmetric with respect to $E = 0eV$ point (see also [30]).

For the case of two nanotubes in parallel contact [29], the distance between nanotubes is fixed to 3.1Å from molecular dynamics simulations. The conductance is not sensitive to small changes in the intertube distance around this value.

Various combinations of metallic nanotubes with different tube size and chirality were investigated. The size of nanotubes is found to have no substantial effect on the conductance, however it depends sensitively on chirality. Shown in Fig. 1 are typical examples of intertube conductance as a function of energy. The best conductance is achieved for *armchair/armchair* or *zigzag/zigzag* configurations. For *armchair/armchair* contacts the conductance can approach that of a perfect nanotube, $4e^2/h$ (Fig. 1 (a)). In contrast, it is an order of magnitude smaller when the two tubes have different chirality(Fig. 1 (c)). This is due to the fact that only *zigzag/zigzag* and *armchair/armchair* contacts allow optimal configurations in which delocalized states are present across the contact (see also Fig 3 (a)). As a function of energy, the

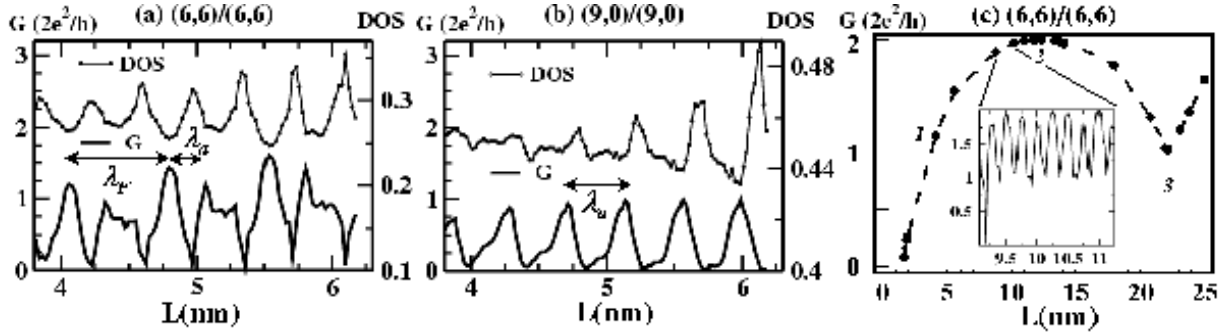

FIG. 2: Conductance and DOS as functions of the contact length at $E = -0.1eV$ for a (a) (6,6)/(6,6) (b) (9,0)/(9,0) parallel contact. Rapid oscillations with a period of unit cell length are present for both armchair($\lambda_a = 2.46$ Å$(= a_0)$) and zigzag ($\lambda_a = 4.26$ Å$(= a_0)$) tubes. Additional modulation related to the Fermi wavelength ($\lambda_F = 3a_0$) can be seen in (a). Due to the fact that $k_F = 0$ for zigzag nanotubes such a modulation is missing in (b)). Notice the correlation between the peaks in the DOS and the minima in the conductance (see the text for discussions). (c) The upper envelope of conduction oscillation as a function of the contact length (L) at $E = -0.1eV$, showing long wavelength oscillation. The maximum conductance can reach that of a perfect nanotube for contact lengths greater than 10nm. Regions labeled by 1, 2, 3 are examined in detail in Fig. 2(a), 3(a), 3(c). The solid dots correspond to calculated local conduction maxima. The insert shows an example of actual dependence of conductance on contact length.

conductance exhibits a series of minima. Examination of electronic structure revealed that these minima correspond to peaks in the density of states (DOS) of the contact region. This suggests that resonant backscattering due to the quasi bound states formed in the contact area is responsible for the conductance dips (see also Fig. 2, 3). Similar effects have been found for nanotubes with defects [28, 31, 32].

When examining the dependence of conductance on the contact length we found two types of characteristic oscillations [Fig. 2]. At atomic length scale rapid oscillation of conductance with the contact length is related to the unit cell length ($a_0 = 2.46$Å for armchair nanotube and $a_0 = 4.26$Å for zigzag nanotube) and is due to the resonant backscattering on the quasibound states [32] (notice the same correlation between minima in conductance and maxima in DOS as in the case of energy dependence). In *armchair/armchair* contacts additional modulation related to the Fermi wavelength is also present [33, 34, 35].

As one continuously increases the contact length, the rapid oscillation in conductance persists. The envelope of the oscillation shows smooth variation with the contact length (Fig. 2 (c)). Initially the maximum conductance increases rapidly with the contact length. The maximum value approaches $4e^2/h$ (value for a perfect tube) for contact lengths of the order of 10nm. This is surprising considering that the number of quasibound states also increases with the contact length. The explanation is that the quasibound states are formed mainly for certain local arrangements of the atoms in the contact area for which the minima in conductance remain indeed very low at any contact length. For other arrangements delocalized states are formed which facilitate the conduction. In such cases the DOS has values close to those of the perfect tube (see also Fig. 3 (a),(b)). Further increase of the contact length shows unexpected long wavelength oscillation in conductance (Fig. 2 (c)). Resonant cavity-like interference is responsible for this interesting feature. To understand this phenomenon better in Fig. 3 we show 2D contour plots of the local density of states (LDOS) as a function of energy and position along the contact for fixed contact lengths. When the conductance is in the vicinity of a global maximum (marked 2 in Fig. 2 (c)) the LDOS is small and smooth along the contact (Fig. 3 (a),(b)) for most energies. In contrast, when the conductance is in the vicinity of a global minimum (marked 3 in Fig. 2 (c)), one can observe a clear interference pattern across the contact area (Fig. 3 (c)), due to the formation of a resonant cavity in such a configuration. Such resonance is very similar to that observed in a recent experiment [36].

In a semiinfinite tube resonant backscattering of the electrons takes place due to the finite end. The incoming wave and the reflected wave interfere producing a set of maxima and minima in the LDOS along the tube. When two nanotubes are in parallel contact, if the interference maxima in the two tubes overlap for a certain energy and contact length, the contact exhibits a resonant cavity-like behavior. A standing wave pattern in the LDOS along the contact can be observed in this case (Fig. 3 (c)) and the conductance has a global minimum (area 3 in Fig. 2 (c), Fig. 3(d)). When the interference maxima in one tube overlap with the minima in the other tube the LDOS in the two tubes are out of phase and the resonant cavity-like behavior is destroyed (Fig. 3 (a), (b)). The electrons can be easily transmitted through the contact, thus high conductance values (area 2 in Fig. 2 (c), Fig. 3(b)).

As a function of the contact length the long wavelength

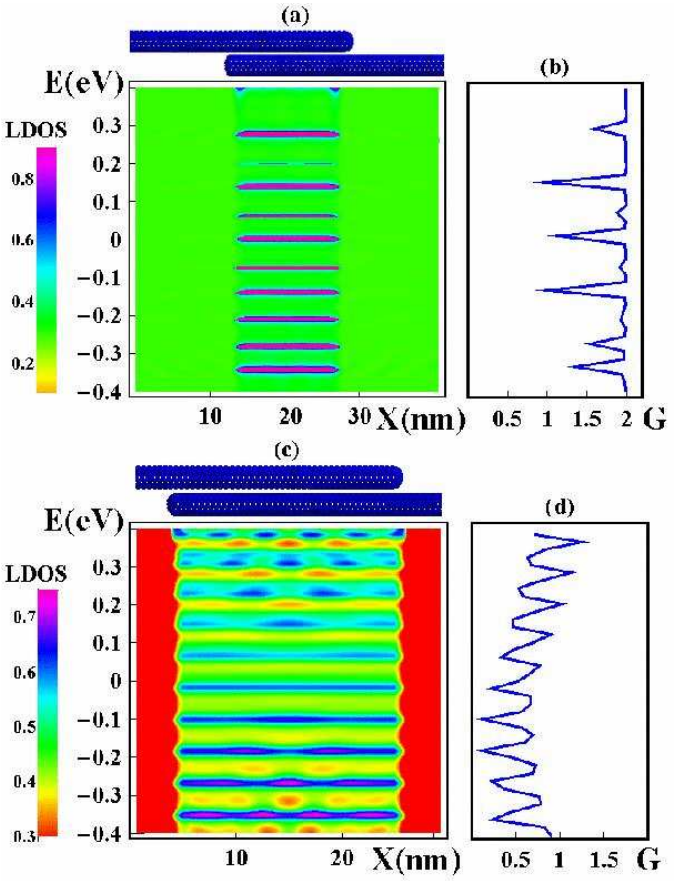

FIG. 3: (a) 2D contour plot of the LDOS (in states/unit cell) along the contact as a function of energy and (b) conductance (in units of $G_0 = 2e^2/h$ as a function of energy for a (6,6)/(6,6) contact when conductance has a global maximum (L=12nm, area 2 in Fig. 2c). Notice that when the conductance is $2G_0$ the LDOS has the same value along the nanotubes and across the contact, indicating the continuation of the conductance band from one tube to the other. (c) 2D contour plot of the LDOS (in states/unit cell) along the contact as a function of energy and (d) conductance (in units of G_0) as a function of energy for a (6,6)/(6,6) contact when conductance has a global minimum (L=22nm, area 3 in Fig. 2c). The standing wave pattern for specific values of the is very clear. The minima in conductance due to formation of quasibound states in the contact area are present in both cases.

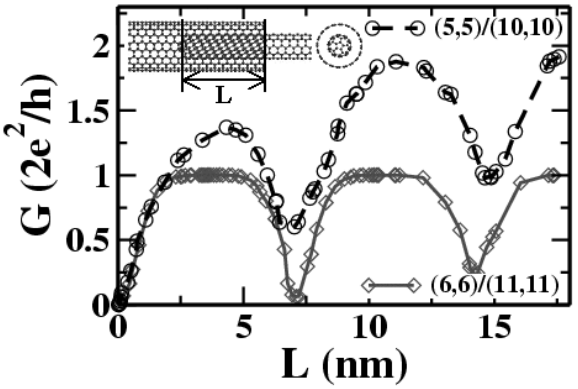

FIG. 4: Envelope function of the conductance for a (5,5)/(10,10) (dotted line) and a (6,6)/(11,11) (full line) concentric geometry contact at $E = -0.1eV$.

oscillation of the conductance depends on the energy: the further the energy is from 0 the smaller is the oscillation wavelength. In a crude approximation we can treat this phenomenon as a beat-like interference between the incoming wave (k_1) and the reflected one (k_2) when they are in different bands, resulting in a modulation of wavelength $\lambda_i = \frac{2\pi}{k_1 - k_2}$. The dispersion relation for the two conduction bands of an armchair nanotube can be written as $\Delta E = \pm V_0(1 - 2\cos\frac{ka}{2})$ [1]. The wave vectors of the electrons located in these bands will be $k_{1,2} = \frac{2}{a}(\frac{\pi}{3} \pm \frac{\Delta E}{V_0\sqrt{3}})$ near Fermi energy, therefore $\lambda_i = \frac{2\pi}{k_1 - k_2} = \frac{3\pi V_0 d}{2\Delta E}$. Thus the wavelength of the long range oscillation should be inverse proportional to the energy. This can be clearly seen in Fig. 3(c) where as one moves away from $E = 0$ the number of maxima increases with the energy across a given contact. Such long range oscillations in LDOS have been observed previously in low dimension electron gas systems [37, 38]. Recent experiments on nanotubes also suggest the existence of such long wave oscillations [25, 28, 36].

The possibility of using multiwall carbon nanotubes as electric circuits components has been suggested since their discovery [39, 40]. Recent experiments show that building devices out of multiwall nanotubes is now possible [41], revealing new potential applications [42]. We considered a contact built from a multiwall nanotube, consisting of two semiinfinite concentric tubes, such that the inner tube can telescope. The dependence of the intertube conductance on the size and the chirality of the tubes was examined. The best conductance is once again achieved by *armchair/armchair* and *zigzag/zigzag* contacts; the other combinations show a conductance at least an order of magnitude smaller. Both atomic scale and long wavelength oscillations are also present. For a given contact length the conductance maxima show a steeper initial increase with the contact length due to the larger contact area of the concentric geometry compared to the parallel case (Fig. 4). The conductance of the contact depends on the intertube distance. The maximum conductance is obtained when the intertube distance d_i is around 3.4Å, the observed interwall distance in multiwall nanotubes[43].

Because in the concentric geometry the symmetry axes of the two nanotubes are aligned the angular momentum is a good quantum number. This means that an electron starting in one of the tubes must scatter to a state with the same symmetry in the other nanotube [12] (this is not the case when the two nanotubes are in parallel contact, as they do not share a common axis and there-

fore angular momentum is not a good quantum number). Considering the case of $(n_1, n_1)/(n_2, n_2)$ nanotube contacts, the two nanotubes have a C_{n_1} and C_{n_2} symmetry respectively. Correspondingly the π bands have the angular quantum number 0 in both tubes [12], while the π^* bands have n_1 and n_2 respectively [44]. As a consequence, the conduction channel due to the π band remains always open while the the conduction channel due to the π^* band is open only if the two nanotubes have compatible rotational symmetry. As an illustration, we show in Fig. 4 the conductance for (5,5)/(10,10) (dotted line) and (6,6)/(11,11) (full line) contacts. In the case of (5,5)/(10,10) contact the $\pi*$ bands have compatible rotational symmetries and the conduction can reach $4e^2/h$. For (6,6)/(11,11) contact the rotational symmetries are incompatible hence the maximum value reached by the conductance is $2e^2/h$. This may explain the observation of only one conductance channel in some multiwall nanotubes experiments [8].

In conclusion, nanotube/nanotube contacts exhibit a variety of novel interesting phenomena. We found that the best conductance is achieved for armchair/armchair and zigzag/zigzag contacts. The conductance maxima increase with the contact length and can reach the value for a perfect tube. For larger contact lengths a long wavelength oscillatory behavior is found. This is attributed to the resonant cavity-like interference phenomena in the contact region. For two concentric nanotubes symmetry breaking can reduce the maximum intertube conductance from $4e^2/h$ to $2e^2/h$. The phenomena discussed here can serve as a foundation for building nanotube electronic circuits and high speed nanoscale electromechanical devices.

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